

Excitations and phase segregation in a two component Bose-Einstein condensate

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Abstract

Bogoliubov-de Gennes (BdG) equations and the excitation spectrum of a two-component Bose-Einstein condensate (BEC) are derived with an arbitrary interaction between bosons, including long-range and short range forces. The nonconverting BEC mixture segregates into two phases for some two-body interactions. Gross-Pitaevskii (GP) equations are solved for the phase segregated BEC. A possibility of boundary-surface and other localised excitations is studied.

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Neutral and charged (Coulomb) Bose-gases became recently of particular interest motivated by the observations of BEC in an alkali vapor [1–5], and by the bipolaron theory of high temperature superconductors [6], respectively. Their theoretical understanding is based on the Bogoliubov [7] displacement transformation, separating a large matrix element of the condensate field operator, $\phi(\mathbf{r}, t)$, from the total $\psi(\mathbf{r}, t)$ and treating the rest $\tilde{\psi}(\mathbf{r}, t) = \psi(\mathbf{r}, t) - \phi(\mathbf{r}, t)$ as a small fluctuation. The resulting (Gross-Pitaevskii) equation for the condensate wave function $\phi(\mathbf{r}, t)$ provides the mean-field description of the ground state and of the excitation spectrum [8–10]. Beyond the mean-field approach the Bogoliubov-de Gennes (BdG)-type equations were derived [11], describing eigenstates of the ‘supra’condensate bosons.

In this letter we extend the Bogoliubov theory to the two-component nonconverting condensate by deriving GP and BdG equations and excitation spectrum with an arbitrary two-body interaction, and solving GP equations for a phase-segregated BEC. Our motivation originates in the recent experimental [5] and theoretical [9,10] studies of BEC of ^{87}Rb atoms in two different hyperfine states, and also in an observation [12] that the condensation temperature of a *two*-component charged Bose gas quantitatively describes the superconducting critical temperature of many cuprates. Differently from Ref. [9,10] we consider nonconverting components (such as different elements), and an arbitrary (rather than short-ranged) two-body interaction.

The Hamiltonian of the two-component (1 and 2) mixture of bosons in an external field with the vector, $A(\mathbf{r}, t)$, and scalar, $U_j(\mathbf{r}, t)$, potentials is given by

$$H = \sum_{j=1,2} \int d\mathbf{r} \psi_j^\dagger(\mathbf{r}) \left[-\frac{(\nabla - iq_j \mathbf{A}(\mathbf{r}, t))^2}{2m_j} + U_j(\mathbf{r}, t) - \mu_j \right] \psi_j(\mathbf{r}) + \frac{1}{2} \sum_{j,j'} \int d\mathbf{r} \int d\mathbf{r}' V_{jj'}(\mathbf{r} - \mathbf{r}') \psi_j^\dagger(\mathbf{r}) \psi_j(\mathbf{r}) \psi_{j'}^\dagger(\mathbf{r}') \psi_{j'}(\mathbf{r}'), \quad (1)$$

where m_j and q_j are the mass, and the effective charge (if any) of the boson j ($\hbar = 1$). If the two-body interactions $V_{jj'}(\mathbf{r})$ are weak, the occupation numbers of one-particle states are not very much different from those in the ideal Bose-gas. In particular the lowest energy state remains to be macroscopically occupied and the corresponding component of the field operator $\psi(\mathbf{r})$ has anomalously large matrix element between the ground states of the system

containing $N + 1$ and N bosons. Hence, it is convenient to consider a grand canonical ansamble, introducing the chemical potentials μ_j to deal with the anomalous averages $\phi(\mathbf{r})$ rather than with the off-diagonal matrix elements. Using the Bogoliubov displacement transformation in the equation of motion for the field operators $\psi(\mathbf{r}, t) = \phi(\mathbf{r}, t) + \tilde{\psi}(\mathbf{r}, t)$ and collecting $c - number$ terms of ϕ , and terms linear in the *supracondensate* boson operators $\tilde{\psi}$ one obtains a set of the GP and BdG-type equations [11,9,10]. The macroscopic condensate wave functions (i.e the order parameters) obey two coupled GP equations

$$i\frac{\partial}{\partial t}\phi_j(\mathbf{r}, t) = \hat{h}_j\phi_j(\mathbf{r}, t) + \sum_{j'} \int d\mathbf{r}' V_{jj'}(\mathbf{r} - \mathbf{r}') |\phi_{j'}(\mathbf{r}', t)|^2 \phi_j(\mathbf{r}, t) \quad (2)$$

with the single-particle Hamiltonian $\hat{h}_j = -(\nabla - iq_j\mathbf{A}(\mathbf{r}, t))^2/2m_j + U_j(\mathbf{r}, t) - \mu_j$. The supracondensate wave-functions satisfy four BdG equations

$$\begin{aligned} \sum_{j'} \int d\mathbf{r}' V_{jj'}(\mathbf{r} - \mathbf{r}') [|\phi_{j'}(\mathbf{r}', t)|^2 u_j(\mathbf{r}, t) + \phi_j^*(\mathbf{r}', t) \phi_{j'}(\mathbf{r}, t) u_{j'}(\mathbf{r}', t) + \\ \phi_j(\mathbf{r}', t) \phi_{j'}(\mathbf{r}, t) v_{j'}(\mathbf{r}', t)] = i\frac{\partial}{\partial t} u_j(\mathbf{r}, t) - \hat{h}_j u_j(\mathbf{r}, t), \end{aligned} \quad (3)$$

and

$$\begin{aligned} \sum_{j'} \int d\mathbf{r}' V_{jj'}(\mathbf{r} - \mathbf{r}') [|\phi_{j'}(\mathbf{r}', t)|^2 v_j(\mathbf{r}, t) + \phi_j(\mathbf{r}', t) \phi_{j'}^*(\mathbf{r}, t) v_{j'}(\mathbf{r}', t) + \\ \phi_j^*(\mathbf{r}', t) \phi_{j'}^*(\mathbf{r}, t) u_{j'}(\mathbf{r}', t)] = -i\frac{\partial}{\partial t} v_j(\mathbf{r}, t) - \hat{h}_j^* v_j(\mathbf{r}, t). \end{aligned} \quad (4)$$

Here we have applied the linear Bogoliubov transformation for $\tilde{\psi}$

$$\tilde{\psi}_j(\mathbf{r}, t) = \sum_n u_{nj}(\mathbf{r}, t) (\alpha_n + \beta_n) + v_{nj}^*(\mathbf{r}, t) (\alpha_n^\dagger + \beta_n^\dagger), \quad (5)$$

where α_n, β_n are bosonic operators annihilating quasiparticles in the quantum state n . There is a sum rule,

$$\sum_n [u_{nj}(\mathbf{r}, t) u_{nj}^*(\mathbf{r}', t) - v_{nj}(\mathbf{r}, t) v_{nj}^*(\mathbf{r}', t)] = \delta(\mathbf{r} - \mathbf{r}'), \quad (6)$$

which retains the Bose commutation relations for all operators.

In the homogeneous system with no external fields the excitation wave functions are plane waves

$$u_{\mathbf{k},j}(\mathbf{r}, t) = u_{\mathbf{k},j} \exp[i\mathbf{k} \cdot \mathbf{r} - iE(\mathbf{k})t], \quad (7)$$

$$v_{\mathbf{k},j}(\mathbf{r}, t) = v_{\mathbf{k},j} \exp[i\mathbf{k} \cdot \mathbf{r} - iE(\mathbf{k})t], \quad (8)$$

The condensate wave function is (\mathbf{r}, t) independent in this case, $\phi_j(\mathbf{r}, t) \equiv \phi_j$. Solving two GP equations one obtains the chemical potentials as

$$\begin{aligned} \mu_1 &= Vn_1 + Wn_2 \\ \mu_2 &= Un_2 + Wn_1, \end{aligned} \quad (9)$$

and solving four BdG equations one determines the excitation spectrum, $E(\mathbf{k})$ from

$$\text{Det} \begin{bmatrix} \xi_1(\mathbf{k}) - E(\mathbf{k}) & V_{\mathbf{k}}\phi_1^2 & W_{\mathbf{k}}\phi_1\phi_2^* & W_{\mathbf{k}}\phi_1\phi_2 \\ V_{\mathbf{k}}\phi_1^{*2} & \xi_1(\mathbf{k}) + E(\mathbf{k}) & W_{\mathbf{k}}\phi_1^*\phi_2^* & W_{\mathbf{k}}\phi_1^*\phi_2 \\ W_{\mathbf{k}}\phi_1^*\phi_2 & W_{\mathbf{k}}\phi_1\phi_2 & \xi_2(\mathbf{k}) - E(\mathbf{k}) & U_{\mathbf{k}}\phi_2^2 \\ W_{\mathbf{k}}\phi_1^*\phi_2^* & W_{\mathbf{k}}\phi_1\phi_2^* & U_{\mathbf{k}}\phi_2^{*2} & \xi_2(\mathbf{k}) + E(\mathbf{k}) \end{bmatrix} = 0. \quad (10)$$

Here $\xi_1(\mathbf{k}) = k^2/2m_1 + V_{\mathbf{k}}n_1$, $\xi_2(\mathbf{k}) = k^2/2m_2 + U_{\mathbf{k}}n_2$, and $V_{\mathbf{k}}, U_{\mathbf{k}}, W_{\mathbf{k}}$ are the Fourier components of $V_{11}(\mathbf{r}), V_{22}(\mathbf{r})$ and $V_{12}(\mathbf{r})$, respectively, $V \equiv V_0, U \equiv U_0, W \equiv W_0$, and $n_j = |\phi_j|^2$ the condensate densities. There are two brunches of excitations with the dispersion

$$E_{1,2}(\mathbf{k}) = 2^{-1/2} \left(\epsilon_1^2(\mathbf{k}) + \epsilon_2^2(\mathbf{k}) \pm \sqrt{[\epsilon_1^2(\mathbf{k}) - \epsilon_2^2(\mathbf{k})]^2 + \frac{4k^4}{m_1m_2}W_{\mathbf{k}}^2n_1n_2} \right)^{1/2}, \quad (11)$$

where $\epsilon_1(\mathbf{k}) = \sqrt{k^4/(4m_1^2) + k^2V_{\mathbf{k}}n_1/m_1}$ and $\epsilon_2(\mathbf{k}) = \sqrt{k^4/(4m_2^2) + k^2U_{\mathbf{k}}n_2/m_2}$ are Bogoliubov's modes of two components. If the interactions are short-ranged (hard-core) repulsions, so that $V_{\mathbf{k}} = V, U_{\mathbf{k}} = U, W_{\mathbf{k}} = W$, the spectrum, Eq.(11) is that of Ref. [10]. In the long-wave limit both brunches are sound-like with the sound velocities

$$s_{1,2} = 2^{-1/2} \left(Vn_1/m_1 + Un_2/m_2 \pm \sqrt{[Vn_1/m_1 - Un_2/m_2]^2 + 4W^2n_1n_2/(m_1m_2)} \right)^{1/2}. \quad (12)$$

The lowest brunch becomes unstable ($s_2 < 0$) if $W > \sqrt{UV}$. When $W = \sqrt{UV}$ this brunch is quadratic in the long-wave limit

$$E_2(\mathbf{k}) = \frac{k^2}{2(m_1m_2)^{1/2}} \sqrt{\frac{Vn_1m_1 + Un_2m_2}{Vn_1m_2 + Un_2m_1}}, \quad (13)$$

If $m_1 = m_2 = m$ it becomes 'collisionless' [10], i.e $E_2(\mathbf{k}) = k^2/2m$.

The finite-ranged interactions drastically change the whole spectrum. In the extreme case of the long-range Coulomb interaction, $V(\mathbf{k}) = 4\pi q_1^2/k^2$, $U(\mathbf{k}) = 4\pi q_2^2/k^2$, and $W(\mathbf{k}) = 4\pi q_1 q_2/k^2$ the upper brunch is the geometric sum of the familiar plasmon modes [13] for $k \rightarrow 0$,

$$E_1(\mathbf{k}) = \sqrt{\frac{4\pi q_1^2 n_1}{m_1} + \frac{4\pi q_2^2 n_2}{m_2}}, \quad (14)$$

while the lowest brunch is

$$E_2(\mathbf{k}) = \frac{k^2}{2(m_1 m_2)^{1/2}} \sqrt{\frac{q_1^2 n_1 m_1 + q_2^2 n_2 m_2}{q_1^2 n_1 m_2 + q_2^2 n_2 m_1}}. \quad (15)$$

Remarkably, this mode is 'collisionless' at *any* charges of the components if $m_1 = m_2$, Fig.1. Physically, it describes neutral oscillations of condensates, when a charge fluctuation in one component is nullified by a charge fluctuation in another component, and the total charge density does not fluctuate. We conclude that while the Coulomb Bose condensate is a superfluid (according to the Landau criterion), mixture of two Coulomb Bose condensates is not. In a more general case the interaction might include both the long-range repulsion and the hard-core interaction as in the case of bipolarons or any other preformed bosonic pairs [6]. Combination of both interactions, i.e. $V_{\mathbf{k}}, U_{\mathbf{k}}, W_{\mathbf{k}} \propto \text{constant} + 1/k^2$ transforms the lowest quadratic mode into the Bogoliubov sound. Hence, two component condensate of bipolarons is a superfluid.

Finally, let us discuss the phase segregated state of the two-component nonconverting mixture with the hard-core interactions when $W > \sqrt{UV}$ [14]. In that case chemical potentials determined in Eq.(9) are no longer correct. Minimizing the free energy with respect to the equilibrium concentration we find the densities $n'_1 = n_1 + \sqrt{U/V} n_2$ and $n'_2 = n_2 + \sqrt{V/U} n_1$ of two separated phases. The phase boundary is described by two coupled one-dimesional GP equations, Eq.(2),

$$\frac{d^2 f_1}{dx^2} + f_1 - f_1^3 - r f_1 f_2^2 = 0, \quad (16)$$

and

$$\kappa \frac{d^2 f_2}{dx^2} + f_2 - f_2^3 - r f_2 f_1^2 = 0. \quad (17)$$

where we introduce two real dimensionless order parameters, $f_1 = \phi_1/\sqrt{n'_1}$ and $f_2 = \phi_2/\sqrt{n'_2}$, and measure length in units of the coherence length $\xi_1 = (2m_1 V n'_1)^{-1/2}$. Parameter $r \equiv W/\sqrt{UV}$ is larger than 1, and $\kappa = m_1 V n'_1/m_2 U n'_2$ is the ratio of two coherence lengths squared. One can solve these equations analytically in the limit $\kappa \rightarrow 0$, where two coherence lengths differ significantly or in the case $r \rightarrow \infty$. In the limit $\kappa \rightarrow 0$ the first term in the second equation is negligible, so that $f_2 = 0$ if $r f_1^2 > 1$, and $f_2 = \sqrt{1 - r f_1^2}$ if $r f_1^2 < 1$. Substituting this solution into the first equation and using $df_1/dx = F(f)$, one can reduce Eq.(16) to an integrable first order differential equation. The solution satisfying the boundary conditions, $f_1 = 1$ at $x = \infty$ and $f_1 = 0$ at $x = -\infty$ is

$$f_1(x) = \Theta(x - x_1) \tanh(x/\sqrt{2}) + \Theta(x_1 - x) \frac{\sqrt{2}}{(r+1)^{1/2} \cosh[(r-1)^{1/2}(x - x_2)]}, \quad (18)$$

$$f_2(x) = \Theta(x_1 - x) \left(1 - \frac{2r}{(r+1) \cosh^2[(r-1)^{1/2}(x - x_2)]} \right)^{1/2}, \quad (19)$$

where $\Theta(x)$ is the Θ -function, $\tanh(x_1/\sqrt{2}) = r^{-1/2}$ and $\cosh[(r-1)^{1/2}(x_1 - x_2)] = \sqrt{2r/(r+1)}$. Interestingly the *largest* coherence length (in our case ξ_1) determines profile of *both* order parameters. The inter-component mutual repulsion (r) only slightly changes the characteristic lengths, as shown in Fig.2.

The quasiparticle eigenstates of the phase segregated condensate are determined by the *inhomogeneous* BdG equations, Eqs.(3,4). Here we restrict the analysis by surface excitations at the boundary between two condensates in the limit $r \rightarrow \infty$. Substituting Eqs.(18,19) into Eqs.(3,4) we obtain 4 coupled linear differential equations. In the limit $r \rightarrow \infty$ the equations are decoupled in pairs, so that one can solve only first two equations at $x > 0$. Integration of the equations near zero provides the boundary condition $u_1(0) = v_1(0) = 0$. Then a simple analysis shows that there are no excitations localised near the boundary in that limit.

This conclusion seems to be quite general for any gapless Bose liquid. For example, one can consider a single component hard-core Bose gas with attractive impurity potential placed at the origin $x = 0$, so that the GP equation is

$$\frac{d^2 f}{dx^2} + f - f^3 + \alpha \delta(x) = 0, \quad (20)$$

where $\alpha > 0$ is the (dimensionless) strength of the potential. The solution is $f(x) = \coth[(|x| + x_0)/\sqrt{2}]$ where $\sinh(x_0/2^{3/2}) = 1/\alpha$. Substituting this solution into the BdG equations Eqs.(3,4) one can see that localised excitations do not appear even in that case. The condensate density increases at $x = 0$ and effectively screens out the attractive potential. However, localised excitations could appear in the gapped Bose-liquid, like the charged Bose gas. In that case they are formed below the plasma frequency.

In conclusion, we have derived the Bogoliubov-de Gennes equations and the excitation spectrum of the two-component Bose-Einstein condensate with an arbitrary interaction between bosons, including long-range and short range forces. Solving GP equations for segregated condensates we found the boundary profile, and showed that localised surface waves do not exist for strongly repulsive components.

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- [14] The condition $W > \sqrt{UV}$, where the lowest branch of the spectrum Eq.(12) becomes unstable, coinsides with the condition, where compressibility of the system becomes negative $|\partial\mu_i/\partial n_j| < 0$. Phase segregation also exists in the case of the *Coulomb + hard – core* interaction. In that case the condition where the spectrum Eq.(11) becomes unstable depends on the plasma frequency. It shows that the higher order corrections to the chemical potential due to the Coulomb interaction are crucial

Figure captions. Fig. 1. The excitation energy spectrum of the two-component BEC with the long-range repulsive and hard-core interactions. In this plot $n_1 = n_2 = n$, $m_1 = m_2$ and $U = V = \omega_p$, $q_1 = q_2 = e$. Different curves correspond to the different values of $W/V = 0.1$ (dashed line), 0.5 (dotted line), and 0.95 (solid line), respectively. Excitation energy is measured in units of the plasma frequency $\omega_p = 4\pi n e^2/m$ and momentum k is measured in invers screening length $q_s = (16\pi e^2 n m)^{1/4}$.

Fig. 2. Density profiles of two phase-separated condensates near the boundary for $r = 2$ (solid line) and $r = 10$ (dotted line), respectively.



